National Center for Computational Sciences Snapshot
The Week of November 12, 2007

Beyond the Valley of Beta Stability
Researchers probe the nature of fleeting nuclei

Not all atomic nuclei are stable—just the ones that last. Most of the elements in the universe are produced by exploding stars known as supernovas; and most of these new nuclei are unbalanced, being far too heavy on the protons or the neutrons and lasting only a tiny fraction of a second.

"What we've found over the last decade is understanding the stable nuclei isn't enough," explained Oak Ridge National Laboratory (ORNL) physicist David Dean. "We know what happens in stable nuclei pretty well—there are only 300 of them—but when you add neutrons to the nucleus, you isolate and amplify different aspects of the underlying interactions within the nucleus."

Dean and a team of researchers from the University of Tennessee (UT), Argonne National Laboratory, and Iowa State University are using the National Center for Computational Sciences' (NCCS's) Cray XT4 Jaguar supercomputer to probe the nature of these fleeting, unstable nuclei in an effort to better understand all nuclei, stable and unstable alike. The team's work ultimately promises to help make nuclear power generation more stable and reliable, as well as to ensure the effectiveness of America's nuclear stockpile. It will also help us understand ourselves and the world in which we live a little better.

Dean discusses his work in upcoming issues of *Physics Today* *, published by the American Institute of Physics, and *SciDAC Review*, published for the Department of Energy.

By pursuing unstable nuclei, the team has expanded its list twentyfold, from around 280 stable nuclei to 6,000 possible nuclei. It is pursuing its calculations on Jaguar with several techniques, depending on the size—and therefore complexity—of the nucleus.

"You get different kinds of physics depending on how many particles you have in the nucleus," Dean said, noting that members of his team are world leaders in nuclear density functional theory. "With just two particles, you never see the kind of effects that you have with 100 particles or 200 particles."

As it moves forward, the team also needs the help of experimental facilities. Physicists are discovering that exotic nuclei far from stability have unexpected properties, and computational scientists must be able to validate their calculations. On the other hand, it is both expensive and time-consuming to explore these nuclei with accelerators.

"At some point you won't be able to do all experiments on nuclei," Dean explained. "What experiments do for you is to enable you to benchmark your theory, to say, 'Ah, I know what my theory is doing in this region.'"

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* David J. Dean, "Beyond the nuclear shell model", Physics Today, vol. 60, pg. 48 (November, 2007)

NCCS Researchers Chosen for Conference
Messer, Mills mull science with the French

Two researchers at the NCCS recently took part in the Young Engineering Scientist Symposium in Washington, D.C. Bronson Messer and Richard Mills were selected for their early career achievements and outstanding research in computational science.

The event, held October 22–24 at the French embassy, gathered 20 young (less than 10 years past their Ph.D.) scientists, 10 from France and 10 from the United States, to brainstorm together for possible collaborative research projects.

"Almost everyone got involved for some initial proposal for a research project," said Messer, whose proposals included projects for preconditioners for linear systems and solvers for magnetohydrodynamics. "It was great to learn about new solver technology, especially avenues that aren't being explored in the U.S.," he added.

Following the conference, a French co-organizer of the event was invited by Thomas Zacharia, associate laboratory director for computing and computational sciences, to visit ORNL.

Sixth Annual Day of Science Delivers
DOE event draws 1,200 students, faculty

Over 1,200 students from 125 colleges and universities descended on the Knoxville Convention Center on Monday, October 29 for the Sixth Annual Day of Science.

The event, sponsored by the Department of Energy and ORNL, was one of the largest DOE educational events ever held and was three times larger than any previous Day of Science, featuring speakers and exhibits from government laboratories and universities aimed at recruiting the next generation of American scientists. While many other nations are witnessing increases in their numbers of young scientists, America is witnessing a steep decline, a trend which the Day of Science hopes to counter. Participants were shown first-hand the latest developments in green energy, nanoscience, fusion, and astrophysics, to name a few.

"Some of the students participating in this event will be making the important scientific discoveries of tomorrow," ORNL Director Thom Mason said. "ORNL is proud to be a major partner in encouraging them to pursue science careers."

Once again, Oak Ridge National Laboratory was well represented at the event, giving future scientists a glimpse at the numerous career opportunities available at the lab.

Among the departments present were the Computer Science and Mathematics Division, the Computer Science and Engineering Division, the Information Technology Services Division, the Computing and Computational Sciences Directorate, the Research Alliance in Math and Science program, and the NCCS.

"This was my second year attending the Day of Science," said Don Frederick, a member of the User Assistance and Outreach Group at the NCCS. "I was impressed by the increased attendance and visibility for the event due to more participation by the Department of Energy and associated laboratories. I was most impressed by meeting with the students ─ their enthusiasm for science and technology was invigorating."

Nearly 70 exhibits lined the halls and rooms of the convention center displaying the latest research in areas as diverse as green energy and astrophysics. Various workshops also educated students on the finer points of scholarships, grants, internships, and employment.

Other research institutions represented include Argonne National Laboratory, Brookhaven National Laboratory, and the Princeton Plasma Physics Laboratory.

Lustre Workshop Held at NCCS
System administrators learn tools, tricks

The NCCS recently held a Lustre systems administration workshop at ORNL. Lustre is a highly scalable file system used on some of the world's fastest supercomputers, including the Jaguar system at the NCCS.

NCCS group leader for Technology Integration Shane Canon led the workshop, which took place October 15 and 16. "The workshop focused on a review of the Lustre file system and how it works and specific details of tools and tricks system administrators can use," said Canon, who has led similar workshops in the past.

The workshop was well attended, said Canon, adding that follow-up workshops will be held in the future.

Zacharia Takes on VP Post at the University of Tennessee
Now UT Vice-President for Science and Technology

Associate Laboratory Director for Computing and Computational Sciences Thomas Zacharia has taken on an additional position at UT. The university announced Monday that he has been named UT Vice-President for Science and Technology.

Zacharia will continue to lead the Computing and Computational Sciences directorate at ORNL.

"This additional role for Thomas represents a significant new milestone for UT-Battelle's management of the Laboratory and for the growing partnership between UT and ORNL," Laboratory Director Thom Mason said in a staff e-mail Monday morning.

UT President John Petersen says the joint appointment marks a new level of participation and integration for the UT–ORNL partnership that enhances the capabilities of both institutions by sharing the expertise of key individuals. UT Executive Vice-President David Millhorn emphasizes computing's growing role in research as a driver in Zacharia's selection.

"At the University of Tennessee, Dr. Zacharia will coordinate efforts to integrate supercomputing into our research programs at the university's various campuses across the state," Millhorn says. "Supercomputing is an increasingly important tool used to solve problems as complex and diverse as those being studied in the fields of health care, engineering, and climate change. Having Dr. Zacharia join UT's senior leadership will strengthen the university's goal of becoming a leader in high-performance computing."

ORNL's computational ties to the university go back decades but gained momentum with the establishment of the Joint Institute for Computational Sciences (JICS), which was the first of four new state-funded joint institutes, and particularly with the recent award to UT of a National Science Foundation–funded supercomputing center, which will be housed at ORNL in JICS.